UC Santa Cruz

Graduate Research Symposium 2018

Title

Property-Based Selection of Membrane Permeable Macrocyclic Scaffolds in a DNA-Encoded Library

Permalink
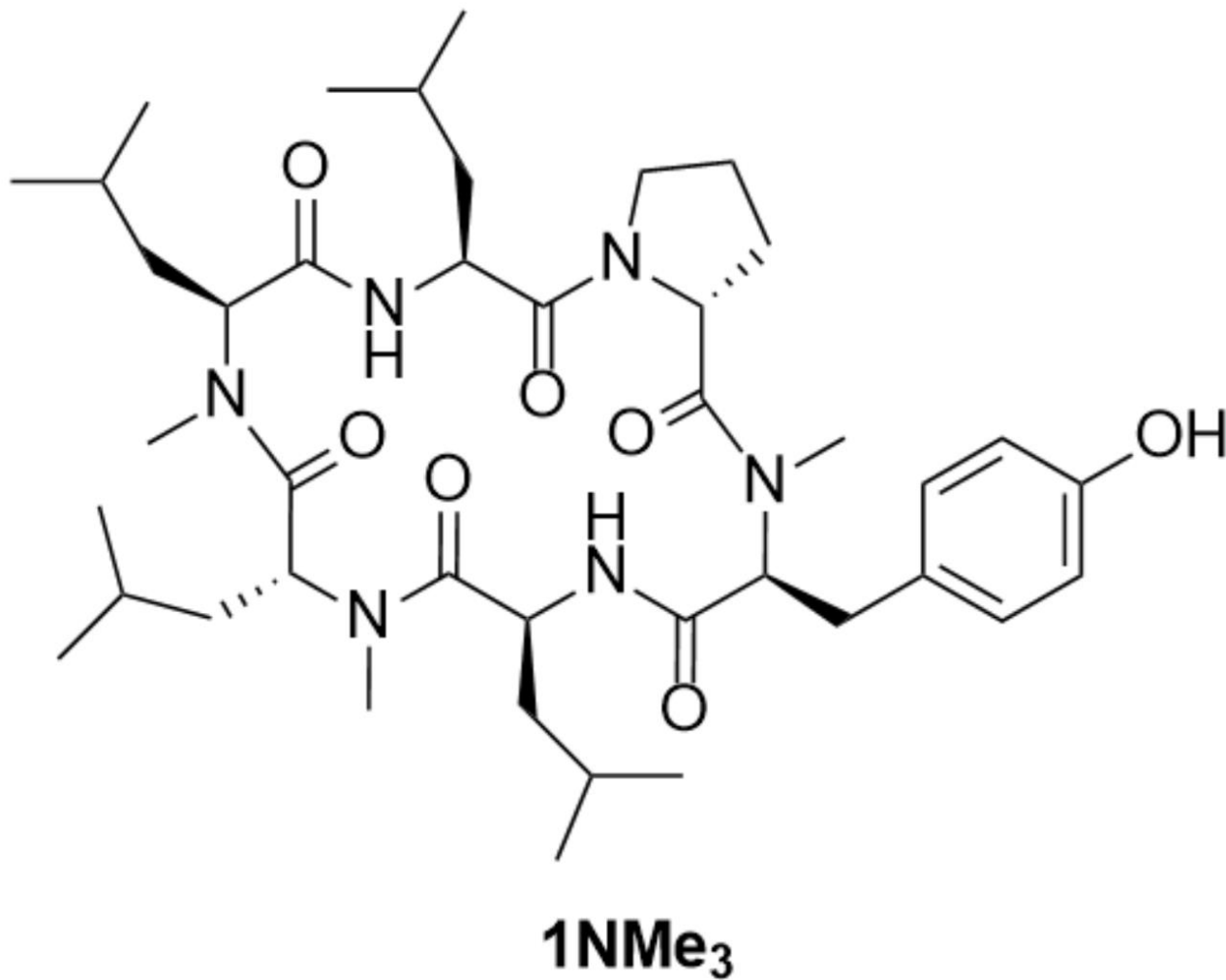
https://escholarship.org/uc/item/37b9s0k8

Author

Koch, Grant Andrew

Publication Date

2018-05-01

Copyright Information

Property-Based Selection of Membrane Permeable Macrocyclic Scaffolds in a DNA-Encoded Library

Grant Koch

UNIVERSITY OF CALIFORNIA SANTA CRUZ

Griselimycin, %F=48

1NMe₃

Able to make many different peptides at once ~ **10^12 libraries**

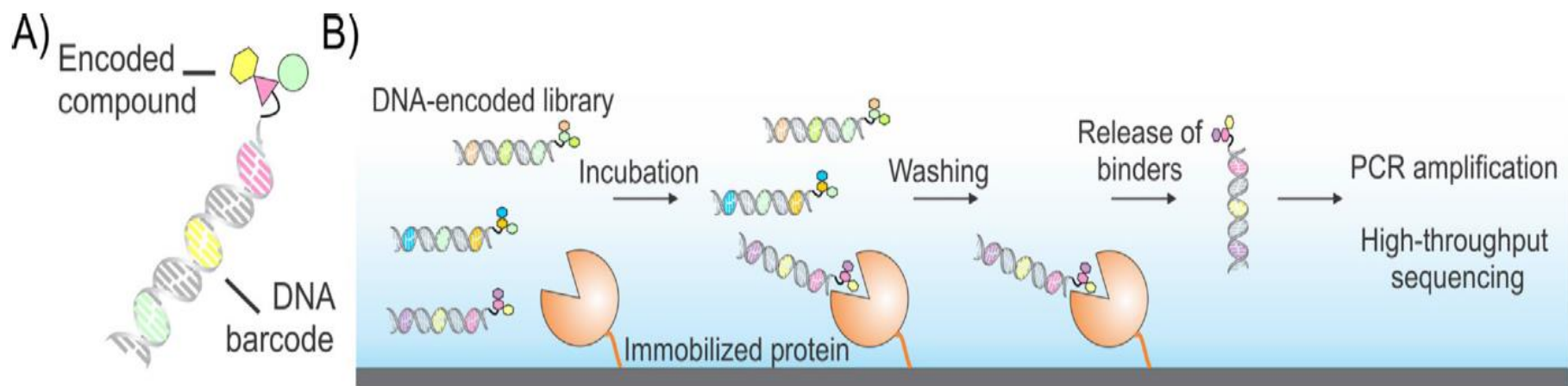# DNA encoded peptides – "Chemical barcoding"
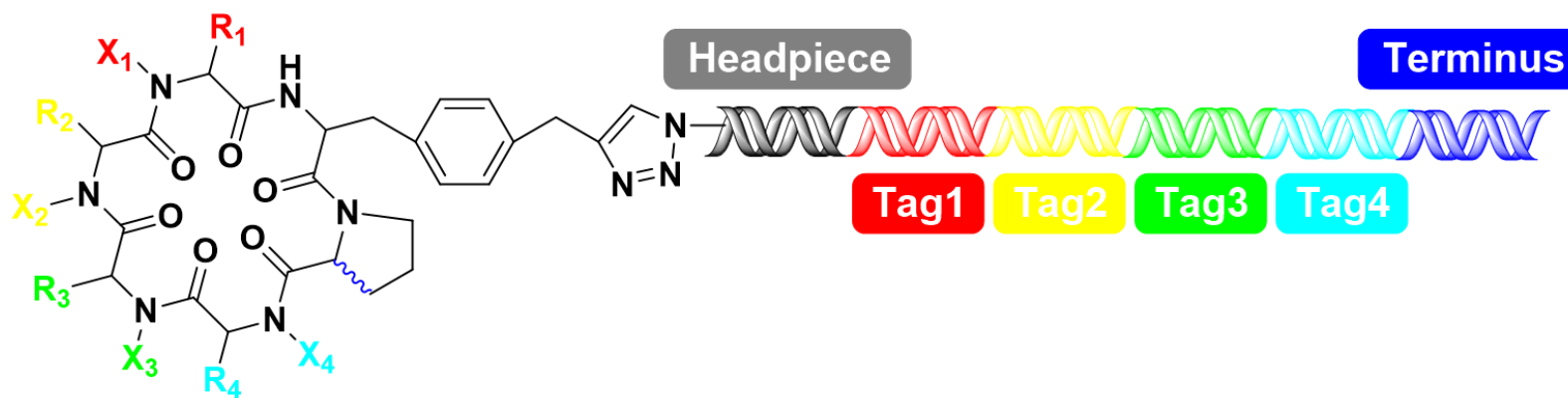
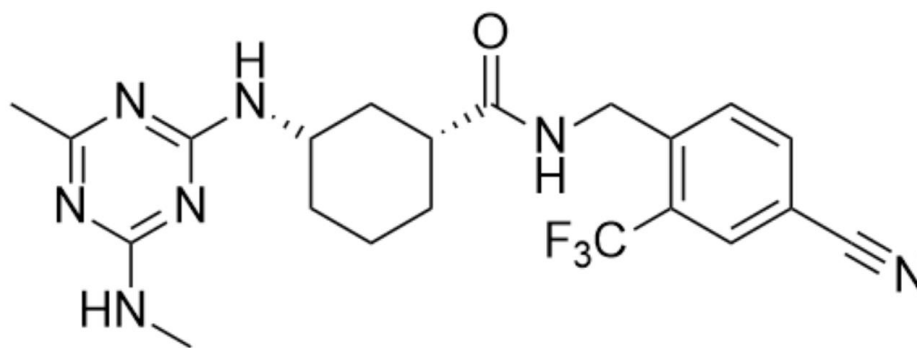**Figure 1.** DNA-encoded chemical libraries (DECLs). A) Generic structure of a DECL. B) Schematic representation of screening protocol.
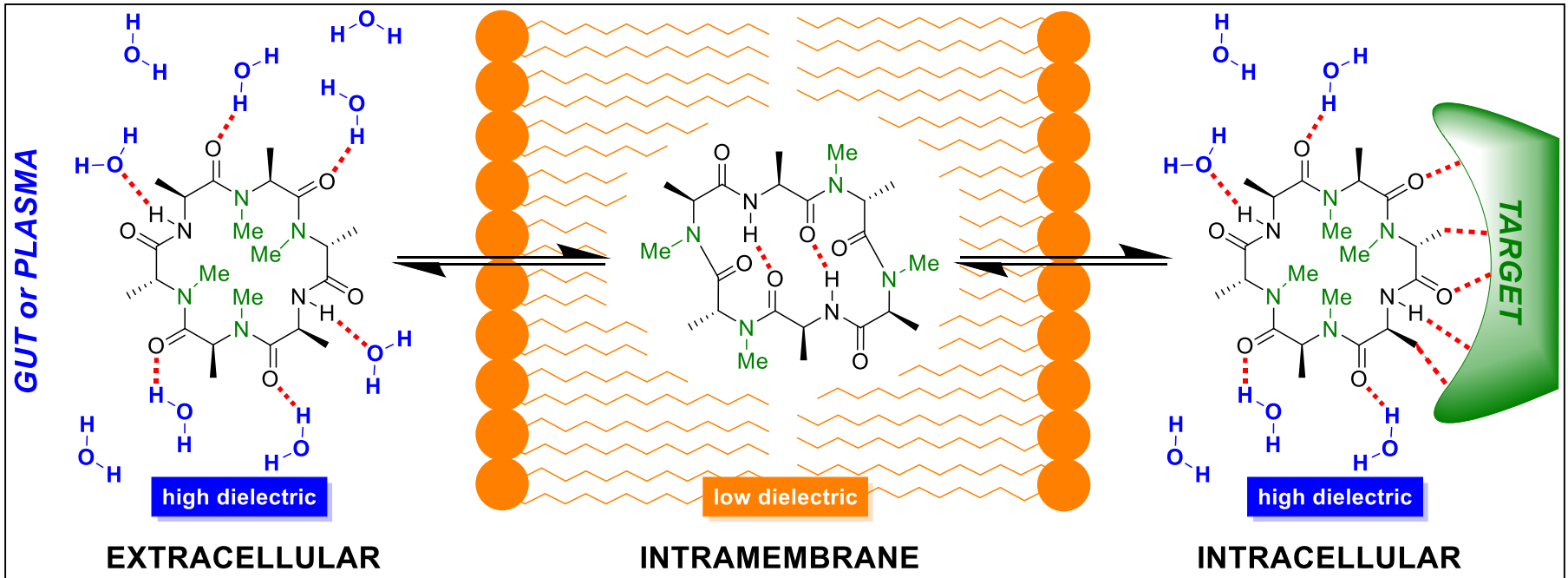
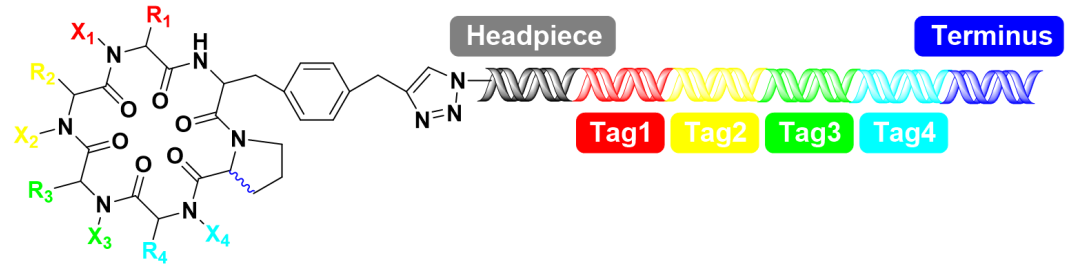*GSK2256294, sEH inhibitor*

Drugs must have:
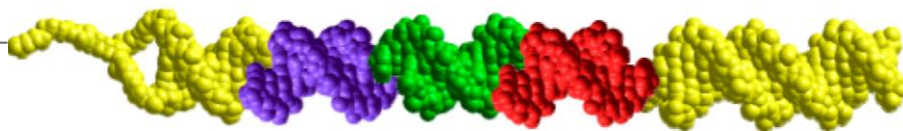- Bioactivity
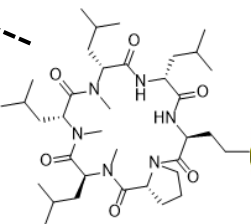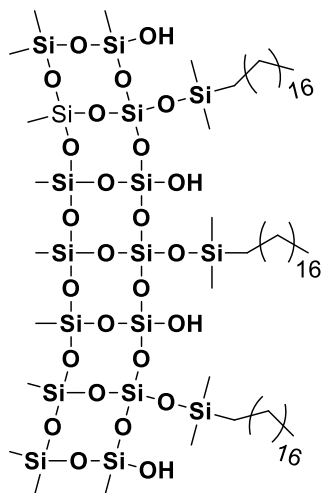- Metabolic stability
- **Cell permeability**

Tightly packed column

HPLC separates mixtures of compounds based on their physical properties

Deng, et al., *ACS* Med. Chem. Lett., 2015

Reverse Phase Alkyl-DNA Separation

$y = 1.0094x + 3.5948$
$R^2 = 0.8747$

WH 6.6

WH 6.7

WH 6.8

WH 6.9